

-- BRIEF DESCRIPTION OF THE DRAWINGS

FIG. 1 shows a first protein crystal packing function histogram utilizing the method of the invention and based on providing the number of possible configurations for a given protein or other molecule of interest with a resolution in Angstroms.

FIG. 2 shows a second protein crystal packing function histogram utilizing the method of the invention and based on providing the number of possible configurations for a given protein or other molecule of interest with a resolution in Angstroms.

FIG. 3 shows a flow chart for the calculation routine of the current invention used to resolve the unphased diffraction amplitudes of the SHSB representations of the current invention.

FIG. 4 shows a space filling schematic for a mathematical representation of the orthorhombic space group of the invention.

FIG. 5 shows a flow chart for the calculation routine of the current invention used to resolve the unphased diffraction amplitudes of the SHSB representations into a Fourier Transformation of the model crystal of the molecule of interest utilizing a fractionalization matrix.

FIG. 6 shows a representation of an Expanded Direct Space Basis Function of the invention.

FIG. 7 shows a representation of a Component Direct Space Basis Function of the invention and the Component Fourier Transformations following there from. --

Analysis of Packing Function Solutions for Monomeric Proteins

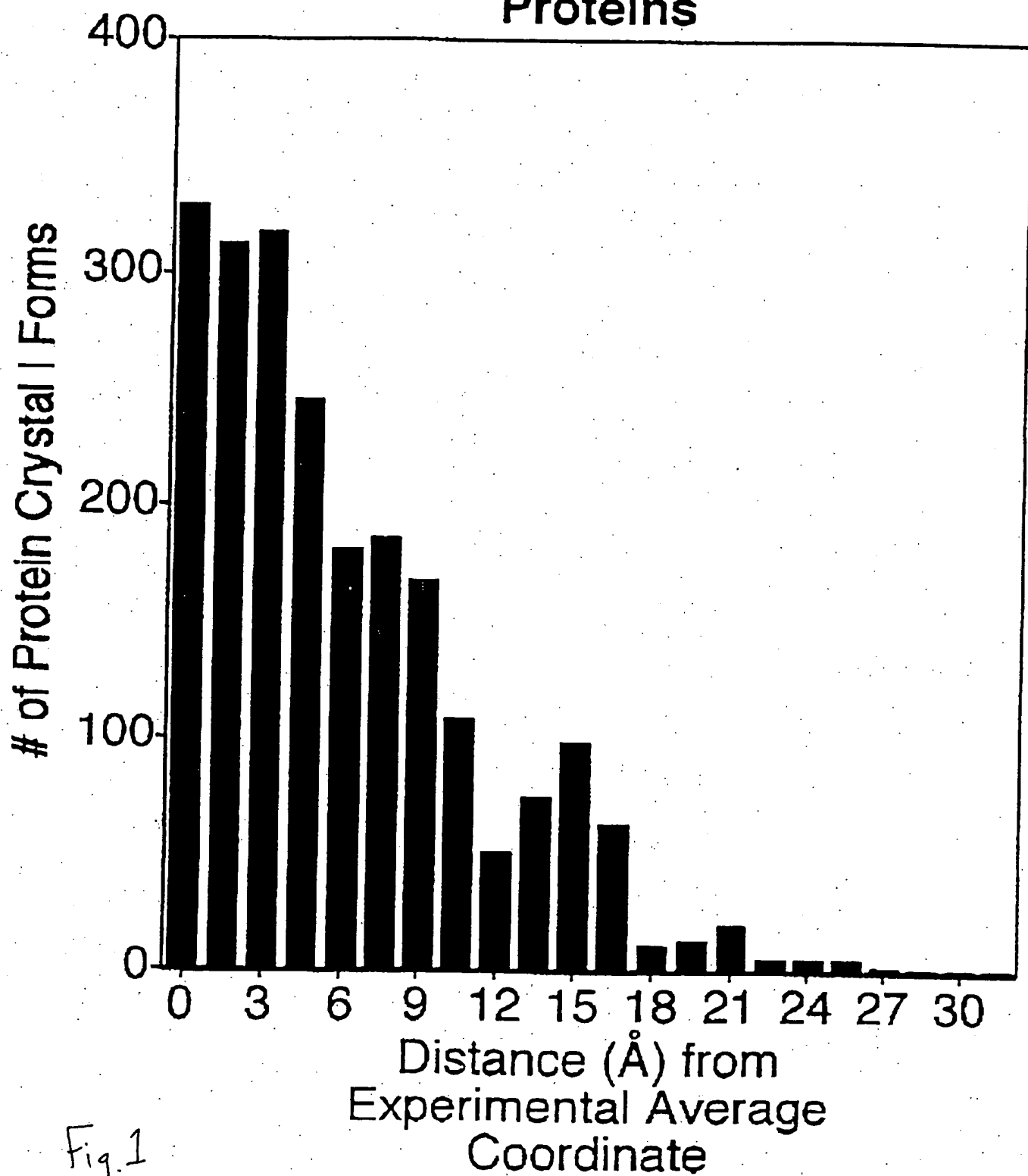


Fig.1

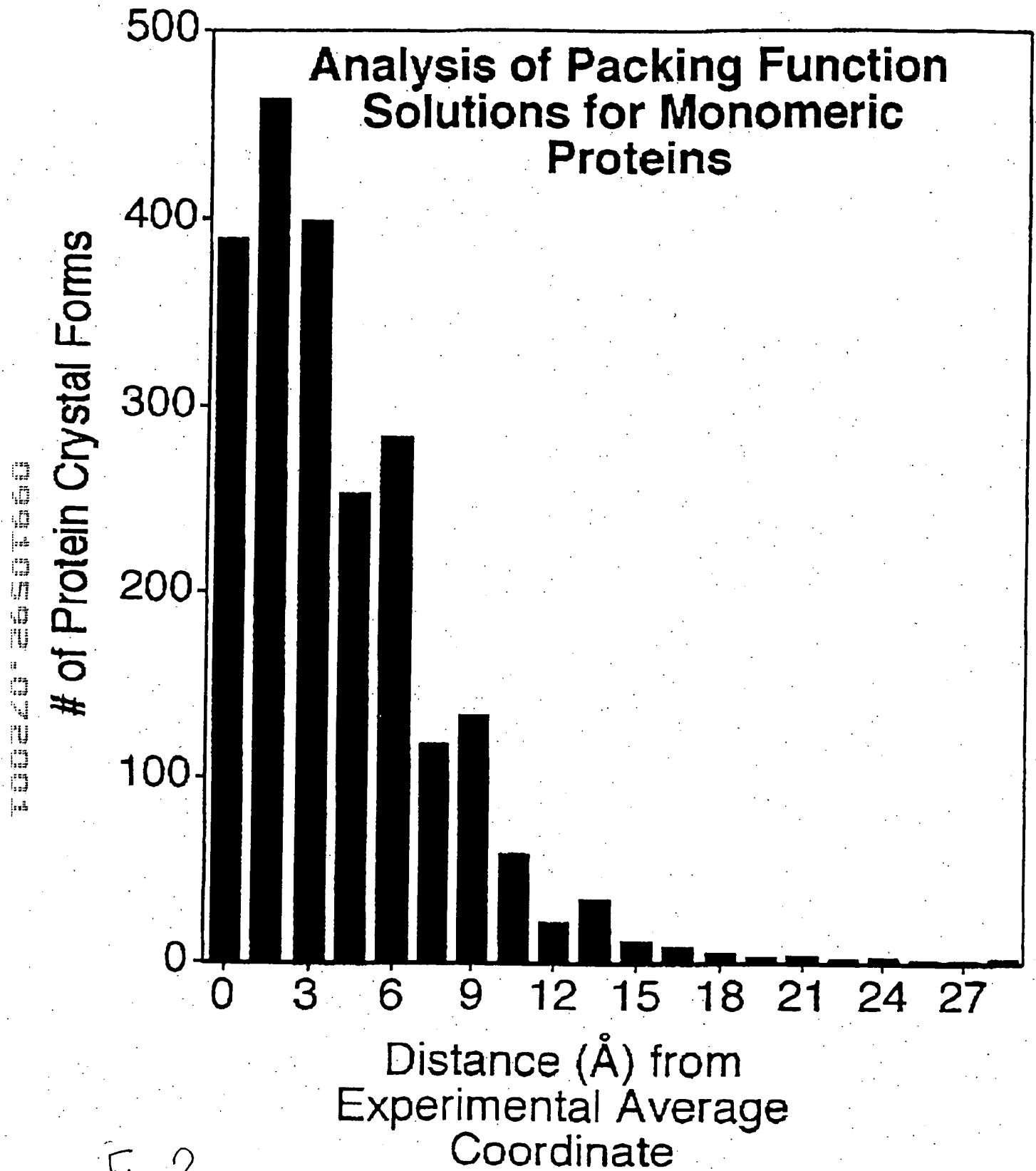


Fig. 2

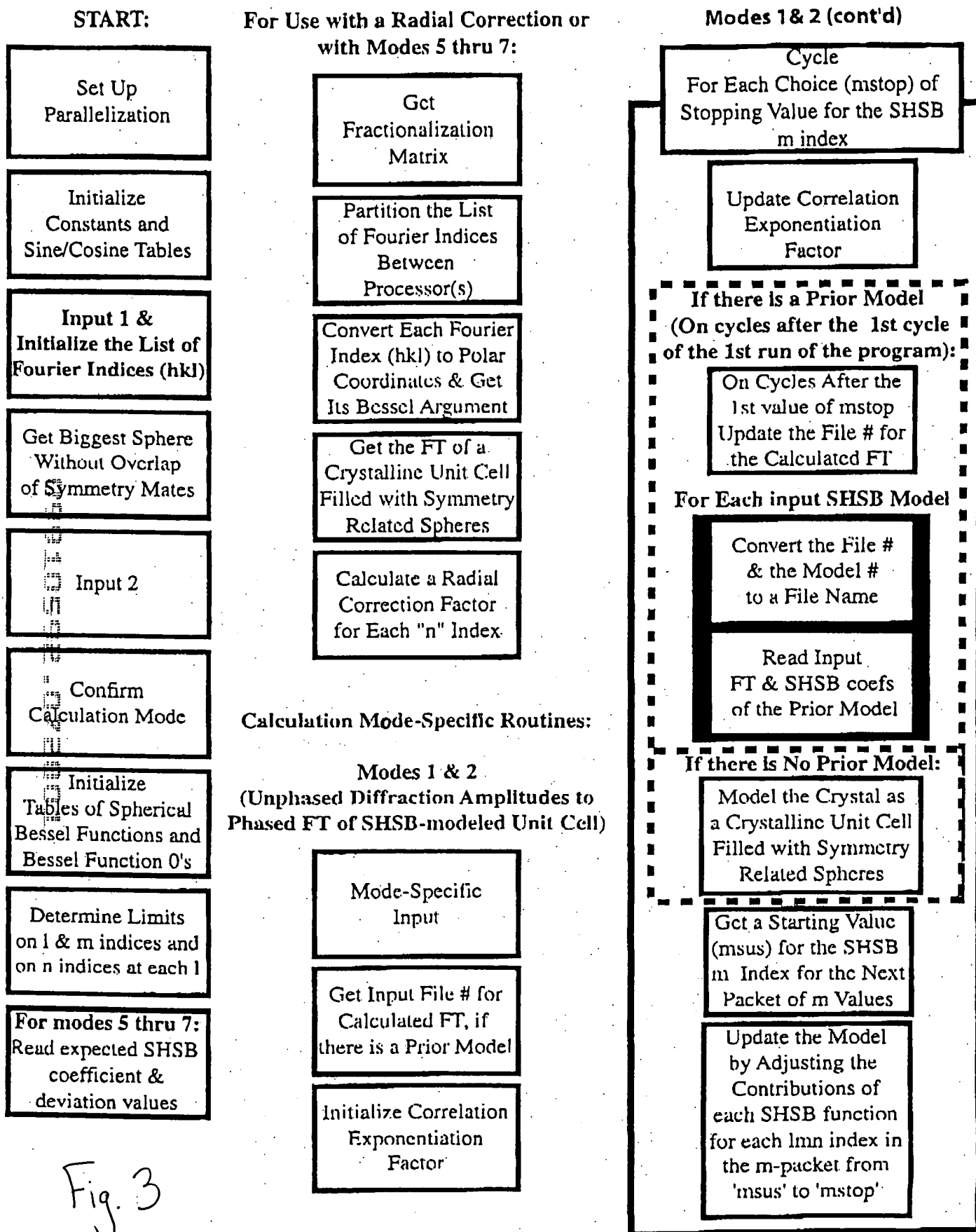


Fig. 3

Flow Chart for the Main Driver Program for "faizer": Options to compute a the FT of a SHSB Model of Crystal

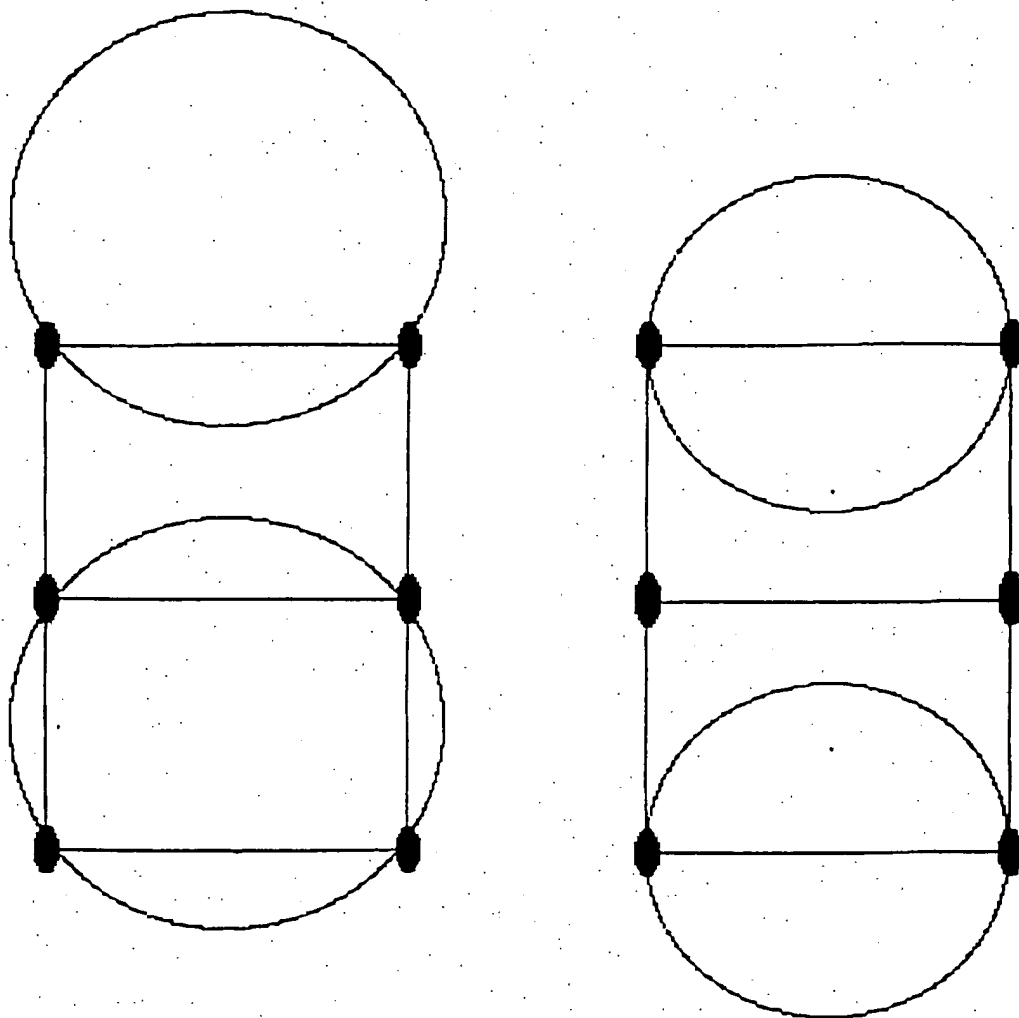


Figure 4 A schematic example; Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals, the local maximum in the packing on the right would be the packing of maximal consistency with the crystallographic data.

Figure 4.

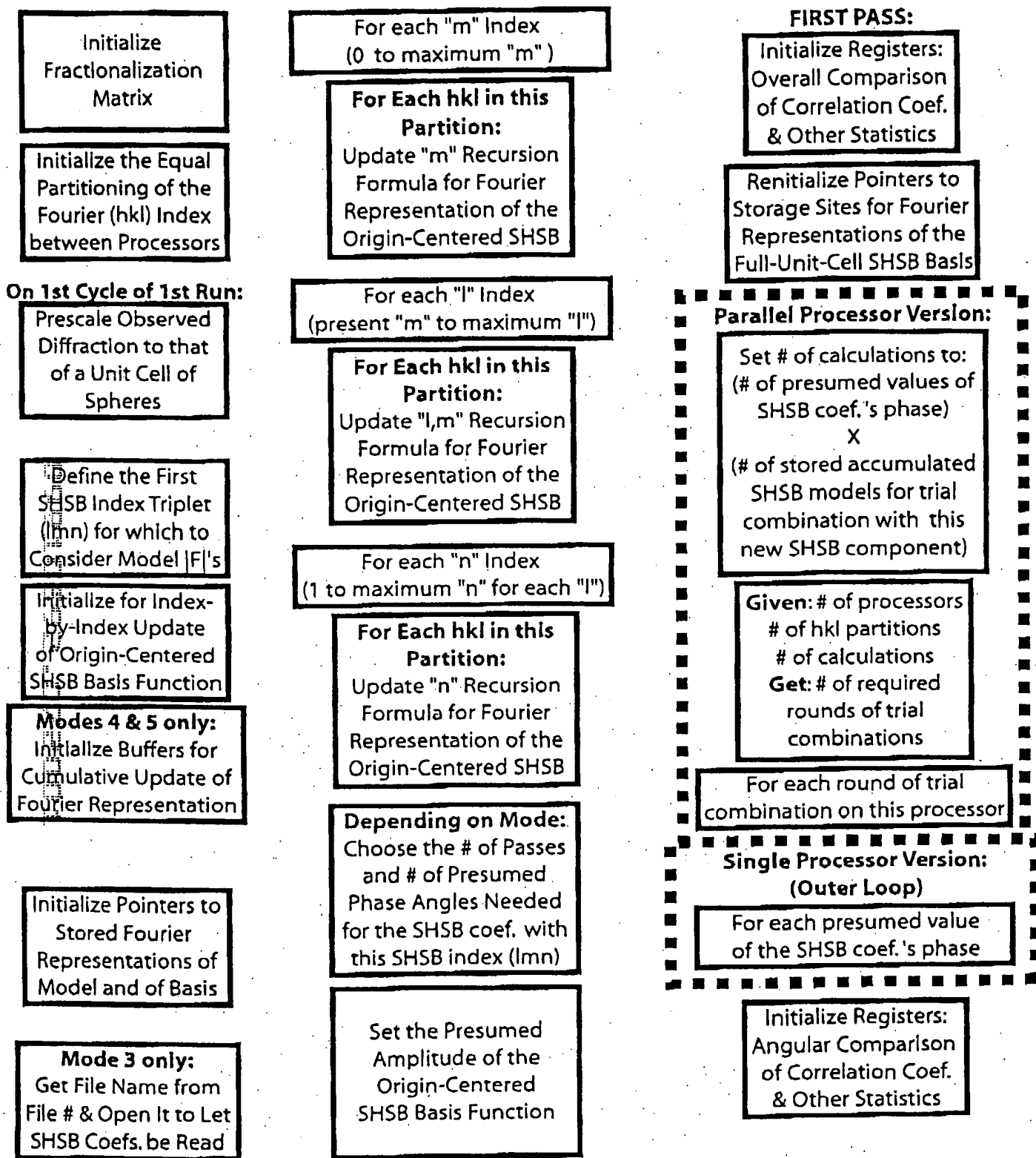
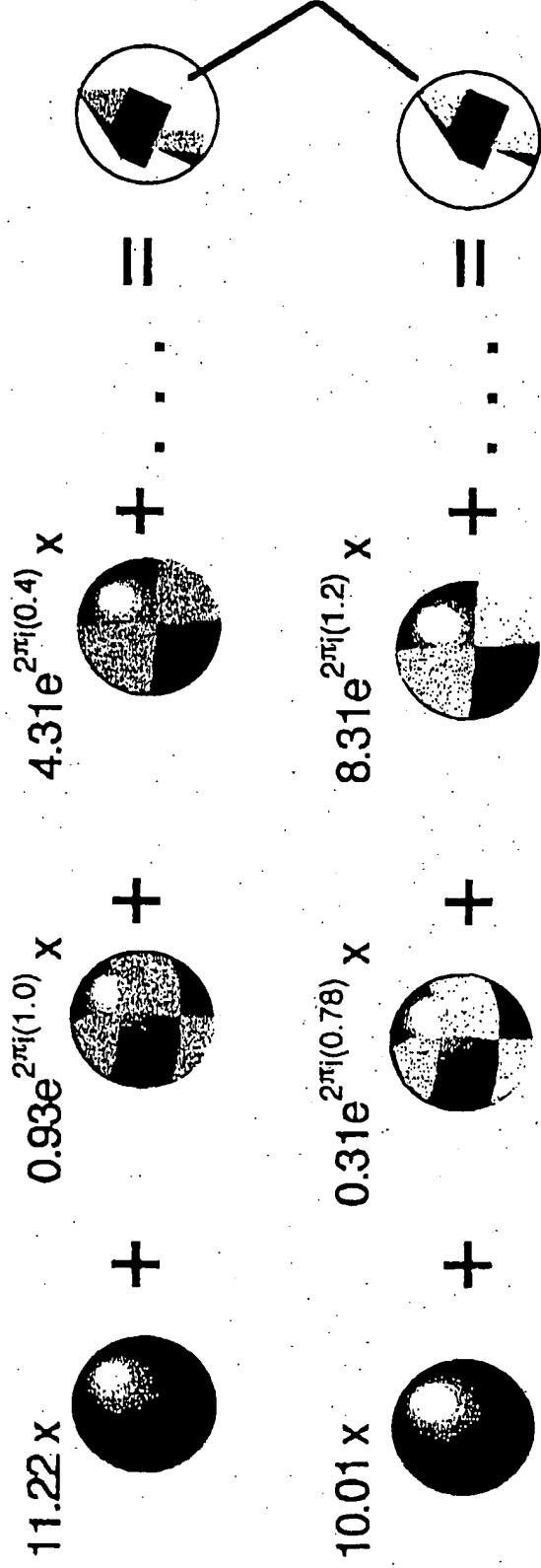


Fig. 5

Identical Image from Expansions about Different Origins:



Symmetry Expanded Direct Space Basis Functions:

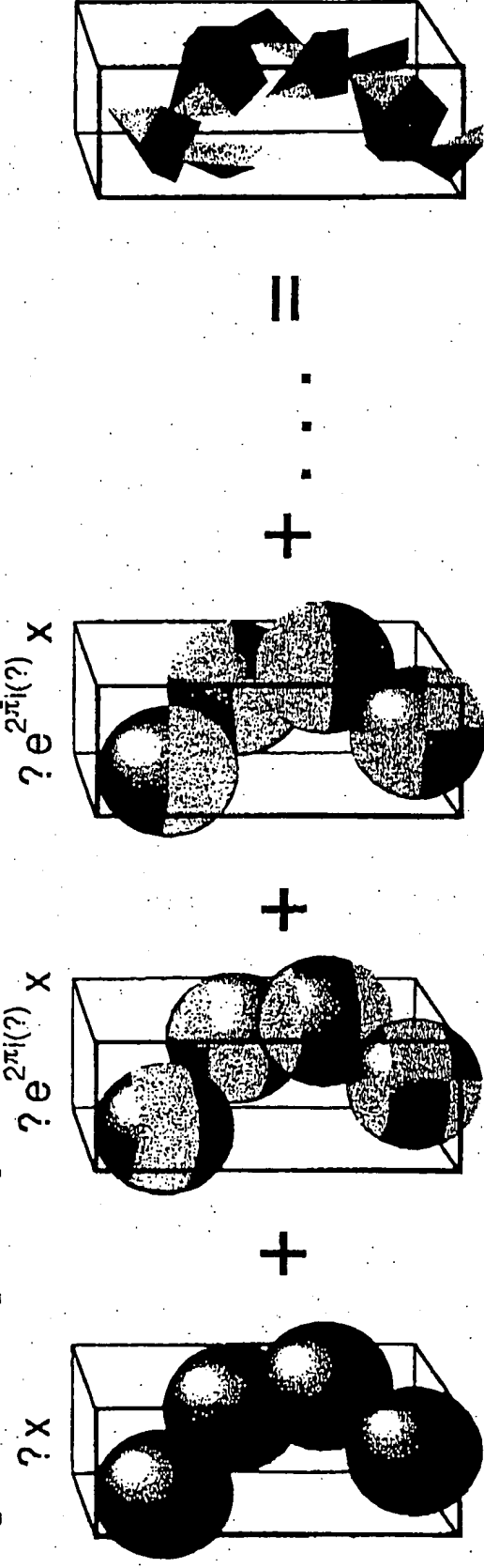
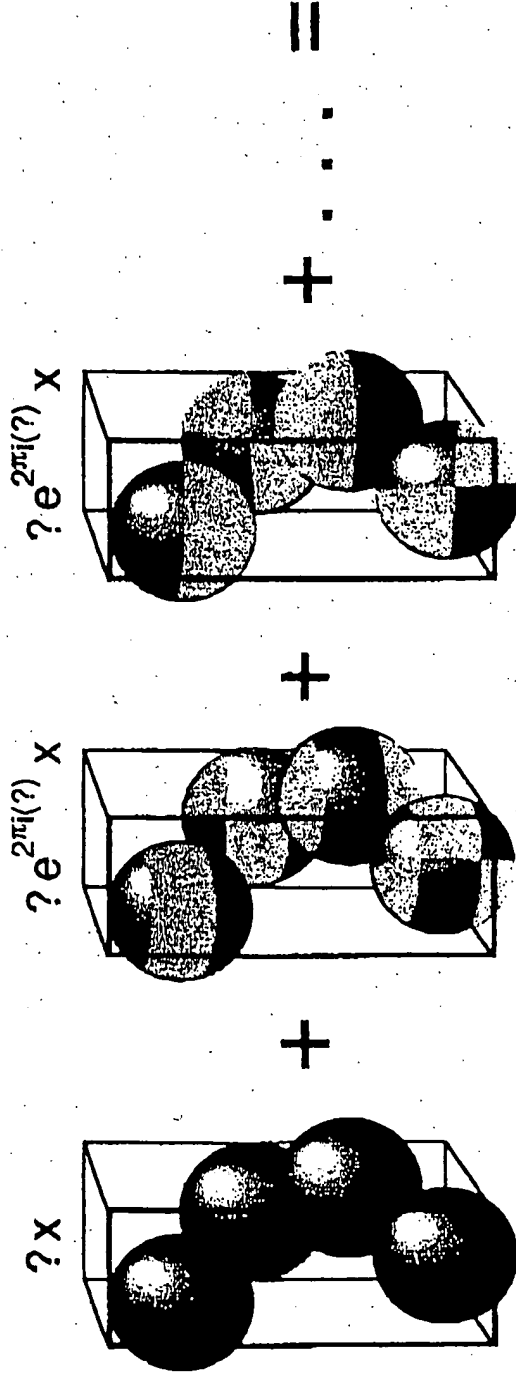


Fig. 6

With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

Component Direct Space Basis Functions:



Component Fourier Transforms:

$$a_{001} F_{\text{solo}}^{001}(hkl) + a_{211} F_{\text{solo}}^{211}(hkl) + a_{111} F_{\text{solo}}^{111}(hkl) + \dots = F_{\text{obs}}(hkl)$$

$$a_{001} = \sum_{hkl} F_{\text{solo}}^{*001}(hkl) F_{\text{obs}}(hkl) \quad [\text{presume } \phi = 0.00 \text{ to start}]$$

$$F_{\text{accum}}(hkl) = a_{001} F_{\text{solo}}^{001}(hkl)$$

$$a_{211} = \sum_{hkl} F_{\text{solo}}^{*211}(hkl) (|F_{\text{obs}}(hkl)| - |F_{\text{accum}}^{n-1}(hkl)|) e^{2\pi i \phi_{\text{accum}}^n(hkl)}$$

$$F_{\text{accum}}^{n+1}(hkl) = F_{\text{accum}}^n(hkl) + a_{211} F_{\text{solo}}^{211}(hkl)$$

Fig. 7